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ON THE WIDOM–ROWLINSON OCCUPANCY FRACTION IN REGULAR GRAPHS

EMMA COHEN, WILL PERKINS, PRASAD TETALI

ABSTRACT. We consider the Widom–Rowlinson model of two types of interacting particles on d -regular graphs. We prove a tight upper bound on the occupancy fraction, the expected fraction of vertices occupied by a particle under a random configuration from the model. The upper bound is achieved uniquely by unions of complete graphs on $d + 1$ vertices, K_{d+1} ’s. As a corollary we find that K_{d+1} also maximises the normalised partition function of the Widom–Rowlinson model over the class of d -regular graphs. A special case of this shows that the normalised number of homomorphisms from any d -regular graph G to the graph H_{WR} , a path on three vertices with a loop on each vertex, is maximised by K_{d+1} . This proves a conjecture of Galvin.

1. THE WIDOM–ROWLINSON MODEL

A *Widom–Rowlinson assignment* or *configuration* on a graph G is a map $\chi : V(G) \rightarrow \{0, 1, 2\}$ so that 1 and 2 are not assigned to neighbouring vertices, or in other words, a graph homomorphism from G to the graph H_{WR} consisting of a path on 3 vertices with a loop on each vertex (the middle vertex represents the label 0). Call the set of all such assignments $\Omega(G)$. The *Widom–Rowlinson model* on G is a probability distribution over $\Omega(G)$ parameterised by $\lambda \in (0, \infty)$, given by:

$$\mathbb{P}[\chi] = \frac{\lambda^{X_1(\chi) + X_2(\chi)}}{P_G(\lambda)},$$

where $X_i(\chi)$ is the number of vertices coloured i under χ , and

$$P_G(\lambda) = \sum_{\chi \in \Omega(G)} \lambda^{X_1(\chi) + X_2(\chi)}$$

is the *partition function*. Evaluating $P_G(\lambda)$ at $\lambda = 1$ counts the number of homomorphisms from G to H_{WR} . We think of vertices assigned 1 and 2 as “coloured” and those assigned 0 as “uncoloured” (see Figure 1).

The Widom–Rowlinson model was introduced by Widom and Rowlinson in 1970 [13], as a model of two types of interacting particles with a hard-core exclusion between particles of different types: colour 1 and 2 represent particles of each type and colour 0 represents an unoccupied site. The model has been studied both on lattices [9] and in the continuum [11, 2] and is known to exhibit a phase transition in both cases.

The Widom–Rowlinson model is one case of a general random model: that of choosing a random homomorphism from a large graph G to a fixed graph H . In the Widom–Rowlinson case, we take $H = H_{\text{WR}}$. Another notable case is H_{ind} , an edge between two vertices,

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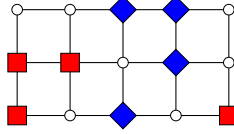


FIGURE 1. A configuration for the Widom–Rowlinson model on a grid. Vertices mapping to 1 and 2 are shown as squares and diamonds, respectively (corresponding to Figure 2).

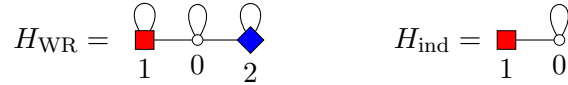


FIGURE 2. The target graphs for the Widom–Rowlinson model and the hard-core model.

one of which has a loop (see Figure 2). Homomorphisms from G to H_{ind} are exactly the independent sets of G , and the partition function of the hard-core model is the sum of $\lambda^{|I|}$ over all independent sets I . An overview of the connections between statistical physics models with hard constraints, graph homomorphisms, and combinatorics can be found in [1].

For every such model, there is an associated extremal problem. Denote by $\text{hom}(G, H)$ the number of homomorphisms from G to H . Then we can ask which graph G from a class of graphs \mathcal{G} maximises $\text{hom}(G, H)$, or if we wish to compare graphs on different numbers of vertices, ask which graph maximises the scaled quantity $\text{hom}(G, H)^{1/|V(G)|}$.

Kahn [8] proved that for any d -regular, bipartite graph G ,

$$(1) \quad \text{hom}(G, H_{\text{ind}}) \leq \text{hom}(K_{d,d}, H_{\text{ind}})^{|V(G)|/2d},$$

where $K_{d,d}$ is the complete d -regular bipartite graph. Equality holds in (1) if G is $K_{d,d}$ or a union of $K_{d,d}$'s. In other words, unions of $K_{d,d}$'s maximise the total number of independent sets over all d -regular, bipartite graphs on a fixed number of vertices.

In a broad generalisation of Kahn's result, Galvin and Tetali [7] showed that in fact, (1) holds for all d -regular, bipartite G and *all* target graphs H (including, for example, H_{WR}). And using a cloning construction and a limiting argument, they showed that in fact the partition function of such models (a weighted count of homomorphisms) is maximised by $K_{d,d}$; for example, for a d -regular, bipartite G ,

$$(2) \quad P_G(\lambda) \leq P_{K_{d,d}}(\lambda)^{|V(G)|/2d},$$

where $P_G(\lambda)$ is the Widom–Rowlinson partition function defined above or the independence polynomial of a graph. Note that the case $\lambda = 1$ is the counting result.

There is no such sweeping statement for the class of all d -regular graphs with the bipartiteness restriction removed. In [14] and [15], Zhao showed that the bipartiteness restriction on G in (1) and (2) can be removed for some class of graphs H , including H_{ind} . But such an extension is not possible for all graphs H ; for example, K_{d+1} has more homomorphisms to H_{WR} than does $K_{d,d}$ (after normalising for the different numbers of vertices). In fact Galvin conjectured the following:

Conjecture 1 (Galvin [5, 6]). *Let G be a any d -regular graph. Then*

$$\text{hom}(G, H_{WR}) \leq \text{hom}(K_{d+1}, H_{WR})^{|V(G)|/(d+1)}.$$

The more general Conjecture 1.1 of [5] that the maximising G for any H is either $K_{d,d}$ or K_{d+1} has been disproved by Sernau [12].

The above theorems of Kahn and Galvin and Tetali are based on the *entropy method* (see [10] and [6] for a survey), but in this context bipartiteness seems essential for the effectiveness of the method. We will approach the problem differently, using the *occupancy method* of [3].

We first define the *occupancy fraction* $\alpha_G(\lambda)$ to be the expected fraction of vertices which receive a (nonzero) colour in the Widom–Rowlinson model:

$$\alpha_G(\lambda) = \frac{\mathbb{E}[X_1 + X_2]}{|V(G)|},$$

where X_i is the number of vertices coloured i by the random assignment χ . A calculation shows that $\alpha_G(\lambda)$ is in fact the scaled logarithmic derivative of the partition function:

$$(3) \quad \alpha_G(\lambda) = \frac{\lambda}{|V(G)|} \cdot \frac{P'_G(\lambda)}{P_G(\lambda)} = \frac{\lambda \cdot (\log P_G(\lambda))'}{|V(G)|}.$$

Our main result is that for any λ , $\alpha_G(\lambda)$ is maximised over all d -regular graphs G by K_{d+1} .

Theorem 2. *Let G be any d -regular graph and $\lambda > 0$. Then*

$$\alpha_G(\lambda) \leq \alpha_{K_{d+1}}(\lambda)$$

with equality if and only if G is a union of K_{d+1} 's.

We will prove this by introducing local constraints on random configurations induced by the Widom–Rowlinson model on a d -regular graph G , then solving a linear programming relaxation of the optimisation problem over all d -regular graphs.

Theorem 2 implies maximality of the normalised partition function:

Corollary 3. *Let G be a d -regular graph and $\lambda > 0$. Then*

$$\frac{1}{|V(G)|} \log P_G(\lambda) \leq \frac{1}{d+1} \log P_{K_{d+1}}(\lambda),$$

or equivalently,

$$P_G(\lambda) \leq P_{K_{d+1}}(\lambda)^{|V(G)|/(d+1)},$$

with equality if and only if G is a union of K_{d+1} 's.

The quantity $\frac{1}{|V(G)|} \log P_G(\lambda)$ is known in statistical physics as the *free energy per unit volume*. Corollary 3 follows from Theorem 2 as follows: $\frac{1}{|V(G)|} \log P_G(0) = 0$ for any G , and so

$$\begin{aligned} \frac{1}{|V(G)|} \log P_G(\lambda) &= \frac{1}{|V(G)|} \int_0^\lambda (\log P_G(t))' dt \\ &\leq \frac{1}{d+1} \int_0^\lambda (\log P_{K_{d+1}}(t))' dt = \frac{1}{d+1} \log P_{K_{d+1}}(\lambda) \end{aligned}$$

where the inequality follows from Theorem 2 and (1). Exponentiating both sides gives Corollary 3.

By taking $\lambda = 1$ in Corollary 3, we get the counting result:

Corollary 4. *For all d -regular G ,*

$$\text{hom}(G, H_{WR}) \leq \text{hom}(K_{d+1}, H_{WR})^{|V(G)|/(d+1)}$$

with equality if and only if G is a union of K_{d+1} 's.

This proves Conjecture 1.

Discussion and related work. The method we use is more probabilistic than the entropy method in the sense that Theorem 2 gives information about an observable of the model; in some statistical physics models, the analogue of $\alpha_G(\lambda)$ would be called the *mean magnetisation*. We also work directly in the statistical physics model, instead of counting homomorphisms.

Davies, Jenssen, Perkins, and Roberts [3] applied the occupancy method to two central models in statistical physics: the hard-core model of a random independent set described above, and the monomer-dimer model of a randomly chosen matching from a graph G . In both cases they showed that $K_{d,d}$ maximises the occupancy fraction over all d -regular graphs. In the case of independent sets this gives a strengthening of the results of Kahn, Galvin and Tetali, and Zhao, while for matchings, it was not known previously that unions of $K_{d,d}$ maximises the partition function or the total number of matchings.

The idea of calculating the log partition function by integrating a partial derivative is not new of course; see for example, the interpolation scheme of Dembo, Montanari, and Sun [4] in the context of Gibbs distributions on locally tree-like graphs. The method is powerful because it reduces the computation of a very global quantity, $P_G(\lambda)$, to that of a locally estimable quantity, $\alpha_G(\lambda)$.

Some partial results towards the Widom–Rowlinson counting problem were obtained by Galvin [5], who showed that a graph with more homomorphisms than a union of K_{d+1} 's must be close in a specific sense to a union of K_{d+1} 's.

2. PROOF OF THEOREM 2

2.1. Preliminaries. To prove Theorem 2, we will use the following experiment: for a d -regular graph G , we first draw a random χ from the Widom–Rowlinson model, then select a vertex v uniformly at random from $V(G)$. We then write our objective function, the occupancy fraction, in terms of local probabilities with respect to this experiment, and add constraints on the local probabilities that must hold for all G . We then relax the optimisation problem to all distributions satisfying the local constraints, and optimise using linear programming.

Fix d and λ . Define a *configuration with boundary conditions* $C = (H, \mathcal{L})$ to be a graph H on d vertices with family of lists $\mathcal{L} = \{L_u\}_{u \in H}$, where each $L_u \subseteq \{1, 2\}$ is a set of allowed colours for the vertex u . Here H represents the neighbourhood structure of a vertex $v \in V(G)$ and the colour lists L_u represent the colours permitted to neighbours of v , given an assignment χ on the vertices outside of $N(v) \cup \{v\}$. (See Figure 3.) Denote by \mathcal{C} the set of all possible configurations with boundary conditions in any d -regular graph.

We now pick the assignment χ at random from the Widom–Rowlinson model on a fixed d -regular graph G , pick a vertex v uniformly at random from $V(G)$, and consider the probability distribution induced on \mathcal{C} .

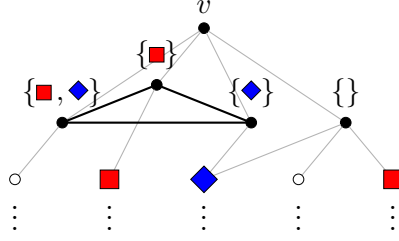


FIGURE 3. An example configuration with boundary conditions based on a colouring χ . The graph H consists of the four neighbours of v along with the black edges, and the list L_u is shown above each vertex u of H . The colours assigned by χ to v and its neighbours are immaterial and so are not shown.

For example, if $G = K_{d+1}$ then with probability 1 the random configuration C is $H = K_d$ with $L_u = \{1, 2\}$ for all $u \in V(H)$. If $G = K_{d,d}$ then H is always d isolated vertices and the colour lists can be any (possibly empty) subset of $\{1, 2\}$, but the lists must be the same for all $u \in V(H)$.

For a configuration $C = (H, \mathcal{L})$, define

$$\alpha_i^v(C) = \mathbb{P}[\chi(v) = i \mid C]$$

$$\alpha_i^u(C) = \frac{1}{d} \sum_{u \in V(H)} \mathbb{P}[\chi(u) = i \mid C],$$

where the probability is over the Widom–Rowlinson model on G given the boundary conditions \mathcal{L} . Note that the spatial Markov property of the model means that these probabilities are “local” in the sense that they can be computed knowing only C . Let $\alpha^v(C) = \alpha_1^v(C) + \alpha_2^v(C)$ and $\alpha^u(C) = \alpha_1^u(C) + \alpha_2^u(C)$. Then we have

$$(4) \quad \alpha_G(\lambda) = \frac{1}{|V(G)|} \sum_{v \in V(G)} \mathbb{P}[\chi(v) \in \{1, 2\}] = \mathbb{E}_C[\alpha^v(C)]$$

$$= \frac{1}{d} \frac{1}{|V(G)|} \sum_{v \in V(G)} \sum_{u \sim v} \mathbb{P}[\chi(u) \in \{1, 2\}] = \mathbb{E}_C[\alpha^u(C)],$$

where the expectations are over the probability distribution induced on \mathcal{C} by our experiment of drawing χ from the model and v uniformly at random from $V(G)$, and the last sum is over all neighbours of v in G . Equality of the two expressions for α follows since sampling a uniform neighbour of a uniform vertex in a regular graph is equivalent to sampling a uniform vertex. We will show that this expectation is maximised when the graph G is K_{d+1} .

We can in fact write explicit formulae for $\alpha^v(C)$ and $\alpha^u(C)$. For a configuration $C = (H, \mathcal{L})$, let $P_C^{(0)}(\lambda)$ be the total weight of colourings of H satisfying the boundary conditions given by the lists \mathcal{L} (corresponding to the partition function for the neighbourhood of v conditioned on $\chi(v) = 0$). Also, write $P_C^{(i)}(\lambda)$ for the total weight of colourings of H satisfying the boundary conditions and using only colour i and 0 (corresponding to the partition functions for the neighbourhood of v conditioned on $\chi(v) = i$). Finally, let $P_C^{(12)}(\lambda) = P_C^{(1)}(\lambda) + P_C^{(2)}(\lambda)$ and let

$$P_C(\lambda) = P_C^{(0)}(\lambda) + \lambda P_C^{(12)}(\lambda)$$

be the partition function of $N(v) \cup \{v\}$ conditioned on the boundary conditions given by C . Note that if \mathcal{L} has a_1 lists containing 1 and a_2 lists containing 2, then $P_C^{(i)}(\lambda) = (1 + \lambda)^{a_i}$.

Now we can write

$$(5) \quad \alpha^v(C) = \frac{\lambda P_C^{(12)}}{P_C} \quad \text{and} \quad \alpha^u(C) = \frac{\lambda \left((P_C^{(0)})' + \lambda (P_C^{(12)})' \right)}{d P_C},$$

where P' is the derivative of P in λ . We will suppress the dependence of the partition functions on λ from now on.

For $G = K_{d+1}$, we have

$$P_{K_{d+1}} = 2(1 + \lambda)^{d+1} - 1$$

$$\alpha_{K_{d+1}}(\lambda) = \frac{2\lambda(1 + \lambda)^d}{2(1 + \lambda)^{d+1} - 1}.$$

If $G = K_{d+1}$ then the only possible configuration is $C_{K_{d+1}}$, the complete neighbourhood K_d with full boundary lists, so we also have $\alpha^u(K_d) = \alpha^v(K_d) = \alpha_{K_{d+1}}(\lambda)$ (we can also compute these directly). Since this quantity will arise frequently, we will use the notation $\alpha_K = \alpha_{K_{d+1}}(\lambda)$.

2.2. A linear programming relaxation. Now let $q : \mathcal{C} \rightarrow [0, 1]$ denote a probability distribution over the set of all possible configurations. Then we set up the following optimisation problem over the variables $q(C)$, $C \in \mathcal{C}$.

$$(6) \quad \alpha^* = \max \sum_{C \in \mathcal{C}} q(C) \alpha^v(C) \quad \text{subject to}$$

$$\sum_{C \in \mathcal{C}} q(C) = 1$$

$$\sum_{C \in \mathcal{C}} q(C) [\alpha^v(C) - \alpha^u(C)] = 0$$

$$q(C) \geq 0 \quad \forall C \in \mathcal{C}.$$

Note that this linear program is indeed a relaxation of our optimisation problem of maximising $\alpha_G(\lambda)$ over all d -regular graphs: any such graph induces a probability distribution on \mathcal{C} , and as we have seen above in (2.1), the constraint asserting the equality $\mathbb{E}\alpha^v(C) = \mathbb{E}\alpha^u(C)$ must hold in all d -regular graphs.

We will show that for any $\lambda > 0$ the unique optimal solution of this linear program is $q(C_{K_{d+1}}) = 1$, where $C_{K_{d+1}}$ is the configuration induced by K_{d+1} : $H = K_d$ and $L_u = \{1, 2\}$ for all $u \in H$.

The dual of the above linear program is

$$\alpha^* = \min \Lambda_p \quad \text{subject to}$$

$$\Lambda_p + \Lambda_c(\alpha^v(C) - \alpha^u(C)) \geq \alpha^v(C) \quad \forall C \in \mathcal{C},$$

with decision variables Λ_p and Λ_c .

To show that the optimum is attained by $C_{K_{d+1}}$, we must find a feasible solution to the dual program with $\Lambda_p = \alpha_K = \frac{2\lambda(1+\lambda)^d}{2(1+\lambda)^{d+1}-1}$. Note that with $\Lambda_p = \alpha_K$ the constraint for $C_{K_{d+1}}$ holds with equality for any choice of Λ_c . In other words, it suffices to find some convex

combination of the two local estimates α^u and α^v which is maximised by $C_{K_{d+1}}$ over all $C \in \mathcal{C}$.

Let C_0 be a configuration with $L_u = \emptyset$ for all $u \in H$ (in which case the edges of H are immaterial, and so abusing notation we will refer to any one of these configurations as C_0). We find a candidate Λ_c by solving the constraint corresponding to C_0 with equality:

$$\begin{aligned}\alpha_K &= \Lambda_c(\alpha^u(C_0) - \alpha^v(C_0)) + \alpha^v(C_0) \\ &= (1 - \Lambda_c) \frac{2\lambda}{1 + 2\lambda}.\end{aligned}$$

This gives

$$\Lambda_c = 1 - \frac{\alpha_K}{2\lambda}(1 + 2\lambda) = \frac{\alpha_K}{2\lambda} \frac{(1 + \lambda)^d - 1}{(1 + \lambda)^d}.$$

With this choice of Λ_c , the general dual constraint is

$$\alpha_K \geq \frac{\alpha_K}{2\lambda} \frac{(1 + \lambda)^d - 1}{(1 + \lambda)^d} \alpha^u(C) + \frac{\alpha_K}{2\lambda} (1 + 2\lambda) \alpha^v(C).$$

Using (2.1), this becomes

$$(7) \quad \frac{(P_C^{(0)})' + \lambda(P_C^{(12)})'}{2P_C^{(0)} - P_C^{(12)}} \leq \frac{d(1 + \lambda)^d}{(1 + \lambda)^d - 1}.$$

From this point on we may assume that C has some non-empty colour list, since otherwise the configuration is equivalent to C_0 and the constraint holds with equality by our choice of Λ_c . This assumption tells us, among other things, that $(P_C^{(0)})' > 0$ and $2P_C^{(0)} - P_C^{(12)} > 0$.

Our goal is now to show that (2.2) holds for all C . We consider the two terms separately.

Claim 5. *For any $C \neq C_0$,*

$$\frac{\lambda(P_C^{(12)})'}{2P_C^{(0)} - P_C^{(12)}} \leq \frac{d\lambda(1 + \lambda)^{d-1}}{(1 + \lambda)^d - 1},$$

with equality if and only if the lists L_u are all equal and C has no dichromatic colourings.

Proof. Since the partition function $P_C^{(0)}$ is at least the total weight $P_C^{(1)} + P_C^{(2)} - 1$ of monochromatic colourings (with equality when C has no dichromatic colourings), we have

$$\frac{(P_C^{(12)})'}{2P_C^{(0)} - P_C^{(12)}} \leq \frac{(P_C^{(12)})'}{P_C^{(12)} - 2} = \frac{a_1(1 + \lambda)^{a_1-1} + a_2(1 + \lambda)^{a_2-1}}{(1 + \lambda)^{a_1} + (1 + \lambda)^{a_2} - 2}$$

(where, as above, a_i is the number of vertices in H allowed colour i under the given boundary conditions), and so we need to show that

$$(8) \quad \frac{a_1(1 + \lambda)^{a_1-1} + a_2(1 + \lambda)^{a_2-1}}{(1 + \lambda)^{a_1} + (1 + \lambda)^{a_2} - 2} \leq \frac{d(1 + \lambda)^{d-1}}{(1 + \lambda)^d - 1}.$$

In general, to show that $(a + b)/(c + d) \leq t$ it suffices to show that $a/c \leq t$ and $b/d \leq t$. Thus it is enough to show that

$$(9) \quad \frac{a(1 + \lambda)^{a-1}}{(1 + \lambda)^a - 1} \leq \frac{d(1 + \lambda)^{d-1}}{(1 + \lambda)^d - 1}$$

whenever $1 \leq a \leq d$. (Note that if either $a_1 = 0$ or $a_2 = 0$ then (2.2) reduces to (2.2), and if both $a_1, a_2 = 0$ then the configuration is C_0). Indeed, it is not hard to check via calculus that the left hand side of (2.2) is increasing with a . This completes the proof of the inequality in Claim 5.

We have equality in this final step when $a_1 = a_2 = d$ or when one is 0 and the other is d . So we have equality overall whenever the lists are all equal and there are no dichromatic colourings (recall that we are assuming C has some non-empty colouring list). \square

Claim 6. *For any $C \neq C_0$,*

$$\frac{(P_C^{(0)})'}{2P_C^{(0)} - P_C^{(12)}} \leq \frac{d(1+\lambda)^{d-1}}{(1+\lambda)^d - 1},$$

with equality if and only if the lists L_u are all equal and C has no dichromatic colourings.

Proof. We can write

$$\begin{aligned} \frac{\lambda(P_C^{(0)})'}{2P_C^{(0)} - P_C^{(12)}} &= \frac{\lambda(P_C^{(0)})'}{P_C^{(0)}} \cdot \frac{P_C^{(0)}}{(P_C^{(0)} - P_C^{(1)}) + (P_C^{(0)} - P_C^{(2)})} \\ &= \frac{\mathbb{E}_C[X_1] + \mathbb{E}_C[X_2]}{\mathbb{P}_C[X_1 > 0] + \mathbb{P}_C[X_2 > 0]}, \end{aligned}$$

where now X_i is the number of vertices coloured i in a random colouring chosen from the Widom–Rowlinson model on C . Noting that $\mathbb{E}_C[X_1] = 0$ whenever $\mathbb{P}_C[X_1 > 0] = 0$, it suffices as above to show that whenever colour 1 is permitted anywhere in C ,

$$(10) \quad \frac{\mathbb{E}_C[X_1]}{\mathbb{P}_C[X_1 > 0]} = \mathbb{E}_C[X_1 \mid X_1 > 0] \leq \frac{\lambda d(1+\lambda)^{d-1}}{(1+\lambda)^d - 1} = \mathbb{E}_{K_d}[X_1 \mid X_1 > 0],$$

and similarly for X_2 , but this will follow by symmetry.

We can decompose the expectation as

$$\mathbb{E}_C[X_1 \mid X_1 > 0] = \sum_{S \subseteq V(H)} \mathbb{P}_C[\chi^{-1}(2) = S \mid X_1 > 0] \cdot \mathbb{E}_C[X_1 \mid X_1 > 0 \wedge \chi^{-1}(2) = S].$$

The partition function restricted to colourings satisfying $X_1 > 0$ and $\chi^{-1}(2) = S$ is just $P_S(\lambda) = \lambda^{|S|}((1+\lambda)^{a_S} - 1)$, where a_S is the number of vertices in $H \setminus S$ which are allowed colour 1 and are not adjacent to any vertex of S . The conditional expectation is then

$$\mathbb{E}_C[X_1 \mid X_1 > 0 \wedge \chi^{-1}(2) = S] = \frac{a_S \lambda (1+\lambda)^{a_S-1}}{(1+\lambda)^{a_S} - 1} \leq \frac{d \lambda (1+\lambda)^{d-1}}{(1+\lambda)^d - 1}$$

with equality precisely when S is empty and 1 is available for every vertex. That is,

$$\mathbb{E}_C[X_1 \mid X_1 > 0] \leq \sum_{S \subseteq V(H)} \mathbb{P}_C[\chi^{-1}(2) = S \mid X_1 > 0] \cdot \frac{d \lambda (1+\lambda)^{d-1}}{(1+\lambda)^d - 1} = \frac{\lambda d (1+\lambda)^{d-1}}{(1+\lambda)^d - 1},$$

as desired. We have equality in (2.2) when $\mathbb{P}_C[a_S = d \mid X_1 > 0] = 1$, which holds for the configurations where 1 is available to every vertex but which have no dichromatic colourings. That is, for equality to hold in the claim C must have no dichromatic colourings, and any colour which is available to some vertex u must be available to every vertex (so the lists must be identical). \square

Adding the inequalities in Claims 6 and 5 shows that (2.2) holds for all C , proving optimality of K_{d+1} .

2.3. Uniqueness.

Lemma 7. *The distribution induced by K_{d+1} is the unique optimum of the LP relaxation (2.2).*

Proof. Complementary slackness for our dual solution says that any optimal primal solution is supported only on configurations C with identical boundary lists and no dichromatic colourings. These fall into three categories:

Case 0: $L_u = \emptyset$ for all u . In this case the edges of H are immaterial, as none of H can be coloured. This is the configuration C_0 above.

Case 1: $L_u = \{i\}$ for all u (for $i = 1$ or 2). The edges of H are again immaterial, as every colouring of H with only colour i is allowed. Call this configuration C_1 .

Case 2: $L_u = \{1, 2\}$ for all u . In this case the prohibition on dichromatic colourings requires that $C = C_{K_{d+1}}$.

We can calculate $\alpha^v(C)$ and $\alpha^u(C)$ for each case. For Case 0 we have

$$\alpha^v(C_0) = \frac{2\lambda}{1+2\lambda} \quad \text{and} \quad \alpha^u(C_0) = 0.$$

For Case 1 we have

$$\alpha^v(C_1) = \frac{\lambda + \lambda(1+\lambda)^d}{\lambda + (1+\lambda)^{d+1}} \quad \text{and} \quad \alpha^u(C_1) = \frac{\lambda(1+\lambda)^d}{\lambda + (1+\lambda)^{d+1}}.$$

And of course, for Case 2 we have

$$\alpha^v(K_d) = \alpha^u(K_d) = \alpha_K.$$

In both Case 0 and Case 1 we have $\alpha^u < \alpha^v$, so the only convex combination q of the three cases giving $\sum_C q(C)\alpha^u(C) = \sum_C q(C)\alpha^v(C)$ (as is required for feasibility) is the one which puts all of the weight on $C_{K_{d+1}}$. \square

3. DISTINCT ACTIVITIES

It is also natural to consider a weighted version of the Widom–Rowlinson model with distinct activities λ_1, λ_2 for the two colours, so that the configuration χ is chosen according to the distribution

$$\mathbb{P}[\chi] = \frac{\lambda_1^{X_1(\chi)} \lambda_2^{X_2(\chi)}}{P_G(\lambda_1, \lambda_2)}$$

where the partition function is

$$P_G(\lambda_1, \lambda_2) = \sum_{\chi \in \Omega(G)} \lambda_1^{X_1(\chi)} \lambda_2^{X_2(\chi)}.$$

We can ask which d -regular graphs maximise $P(\lambda_1, \lambda_2)^{1/|V(G)|}$.

Conjecture 8. *For any $\lambda_1, \lambda_2 > 0$, and any d -regular graph G ,*

$$(11) \quad P_G(\lambda_1, \lambda_2) \leq P_{K_{d+1}}(\lambda_1, \lambda_2)^{|V(G)|/(d+1)}.$$

Now denote by $\alpha_G^1(\lambda_1, \lambda_2)$ and $\alpha_G^2(\lambda_1, \lambda_2)$ the expected fraction of vertices of G that receive colours 1 and 2 respectively in this model.

Conjecture 9. *For any $\lambda_1, \lambda_2 > 0$, the weighted occupancy fraction*

$$\bar{\alpha}_G(\lambda_1, \lambda_2) = \frac{\lambda_2 \alpha_G^1(\lambda_1, \lambda_2) + \lambda_1 \alpha_G^2(\lambda_1, \lambda_2)}{\lambda_1 + \lambda_2}$$

is maximised over all d -regular graphs by K_{d+1} .

In fact, Conjecture 9 implies Conjecture 8. To see this, assume $\lambda_1 \geq \lambda_2$, and let $F_G(x) = \frac{1}{n} \log P_G(\lambda_1 - \lambda_2 + x, x)$. We have

$$\frac{1}{n} \log P_G(\lambda_1, \lambda_2) = F_G(\lambda_2) = F_G(0) + \int_0^{\lambda_2} \frac{dF_G}{dx}(x) dx$$

$F_G(0) = \frac{1}{n} \log P_G(\lambda_1 - \lambda_2, 0) = \log(1 + \lambda_1 - \lambda_2)$ for all graphs G , and so if we can show that for all $0 \leq x \leq \lambda_2$, $\frac{dF_G}{dx}(x)$ is maximised when $G = K_{d+1}$, then we obtain (the log of) inequality (8). We compute:

$$\begin{aligned} \frac{dF_G}{dx}(x) &= \frac{1}{n} \frac{\frac{d}{dx} P_G(\lambda_1 - \lambda_2 + x, x)}{P_G(\lambda_1 - \lambda_2 + x, x)} \\ &= \frac{1}{n} \frac{\sum_{\chi} \frac{x X_1 + (\lambda_1 - \lambda_2 + x) X_2}{x(\lambda_1 - \lambda_2 + x)} (\lambda_1 - \lambda_2 + x)^{X_1} \cdot x^{X_2}}{P_G(\lambda_1 - \lambda_2 + x, x)} \\ &= \frac{1}{x(\lambda_1 - \lambda_2 + x)} \frac{1}{n} \frac{\sum_{\chi} (x X_1 + (\lambda_1 - \lambda_2 + x) X_2) (\lambda_1 - \lambda_2 + x)^{X_1} \cdot x^{X_2}}{P_G(\lambda_1 - \lambda_2 + x, x)} \\ &= \frac{1}{x(\lambda_1 - \lambda_2 + x)} \left[x \alpha_G^{(1)}(\lambda_1 - \lambda_2 + x, x) + (\lambda_1 - \lambda_2 + x) \alpha_G^{(2)}(\lambda_1 - \lambda_2 + x, x) \right]. \end{aligned}$$

Conjecture 9 implies that this is maximised by K_{d+1} .

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